Supporting Information

The Effect of Water upon Deep Eutectic Solvent Nanostructure: An Unusual Transition from Ionic Mixture to Aqueous Solution

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Supporting Information

1. Preparation of hydrated and isotopically-substituted reline samples

Choline chloride (≥99%) was obtained from Fisher, and urea (≥99%) was obtained from Sigma-Aldrich. d_4-urea (CO(ND)$_2$, 99.6% chemical purity, 99.8 atom-% D), and d_9-choline chloride ((CD$_3$)$_3$N(CH$_2$)$_2$OHCl, ≥99% chemical purity) were sourced from QMX laboratories. All chemicals were used as provided. Pure reline samples were first prepared by the literature route of mixing the two desired isotopes in the eutectic molar ratio, followed by heating at 60 ˚C with regular agitation. Water (Elga, 18.2 MΩ) or D$_2$O (Sigma-Aldrich, ≥99.9% chemical purity and atom-% D) was then added to create a series of five choline chloride:urea:water isotope substitutions of H:H:H, H:D:D, D:H:D, D:D:H, and D:D:D. These isotope-substituted ternary DES-water mixtures were prepared in a series of DES:water molar ratios (defined as w), that are described in Table 1.

Table 1. The series of DES sample compositions that were used in these experiments.

Mixture	ChCl:U:W ratio	Water / mol.%	[a]Water / wt.%
Reline-1w	1:2:1	25.0	6.48
Reline-2w	1:2:2	40.0	12.18
Reline-5w	1:2:5	62.5	25.74
Reline-10w	1:2:10	76.9	40.95
Reline-15w	1:2:15	83.3	50.98
Reline-20w	1:2:20	87.0	58.10
Reline-30w	1:2:30	90.9	67.53

[a] The calculated weight percentage here is relevant only for 'normal' hydrogenous DES, and is a variable when the system is deuterium-substituted.

2. Neutron diffraction experiments

Neutron diffraction experiments were performed using different, yet largely analogous instruments. Samples of reline-1w, reline-2w, reline-15w and reline-20w were measured using the SANDALS diffractometer (beamtime allocations RB1510465 and RB1620479), located at TS1 of the STFC ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Harwell, UK. SANDALS is optimised for disordered light-element systems, using time-of-flight (TOF) neutrons with wavelength $0.05 \leq \lambda \leq 4.5$ Å, and a forward scattering detector geometry spanning an angular range of 3.8 - 35.4°, to give a Q-range of $0.1 \leq Q \leq 50$ Å^{-1}. The NIMROD diffractometer, located in TS2 of the same ISIS facility was also used (beamtime allocations RB1610312 and RB1620479) to measure reline-1w, reline-2w, reline-5w, reline-10w, and reline-30w. With a wide neutron TOF spectral range of $0.05 \leq \lambda \leq 11$ Å facilitated by the 100 ms pulse width of the 10 Hz TS2 source,[1] and detectors across the angular range 0.6 – 37.5°, NIMROD gives a wider Q-range than SANDALS. This wide Q-range of $0.01 \leq Q \leq 50$ Å^{-1} facilitates measurement of larger structures, and would therefore allow the microscale phase separation suggested by D'Agostino et al. to be fully characterised.[2] When measurements were taken using both instruments, the results were functionally identical because no small-angle scattering signal was observed. For maximum consistency, SANDALS datasets were therefore used for EPSR modelling only when no NIMROD dataset was available (reline-15w and reline-20w), but instrumental similarity means that this has no bearing on the results.

For both instruments null-scattering, vacuum-sealed Ti$_{0.68}$Zr$_{0.32}$ sample cells with a path-length of 1 mm were filled with around 1.5 g of each sample, before being placed in a sample changer. The evacuated sample environment was regulated to 303 ± 0.1 K using a Julabo recirculating water/ethylene glycol temperature controller. Measurements were performed using a circularly-collimated neutron beam of 30 mm diameter, with a counting time of approximately 8 hours on SANDALS, or 2 hours on NIMROD. Empty sample cells, the empty instrument, and a 3 mm thick vanadium standard were also measured for data normalisation and instrument calibration. Data were processed using GudrunN software.[3] This involved adding corrections for attenuation, multiple scattering and the sample environment background, and normalising the data using the vanadium standard measurement. After a final correction for hydrogen inelasticity, a series of datasets are produced that can be analysed using Empirical Potential Structure Refinement (EPSR) modelling.

In each case, the accurate mass of each sample was recorded (weighing error ± 0.1 mg) in order to determine the sample purity. This was achieved by comparing the measured neutron scattering differential cross section (DCS) with the calculated DCS from the sample masses, using GudrunN neutron total scattering data reduction software.[3] Sample purity was determined to be adequate, as assessed by being within a neutron DCS error margin of $\pm 2\%$ for fully deuterated samples, and $\pm 10\%$ for fully hydrogenous samples. This is within the error of the diffraction experiment and sample preparation, with a higher error for more proton-rich samples because of the strong inelastic scattering of neutrons by hydrogen nuclei.[4] The experimental datasets are shown in Figure 1.
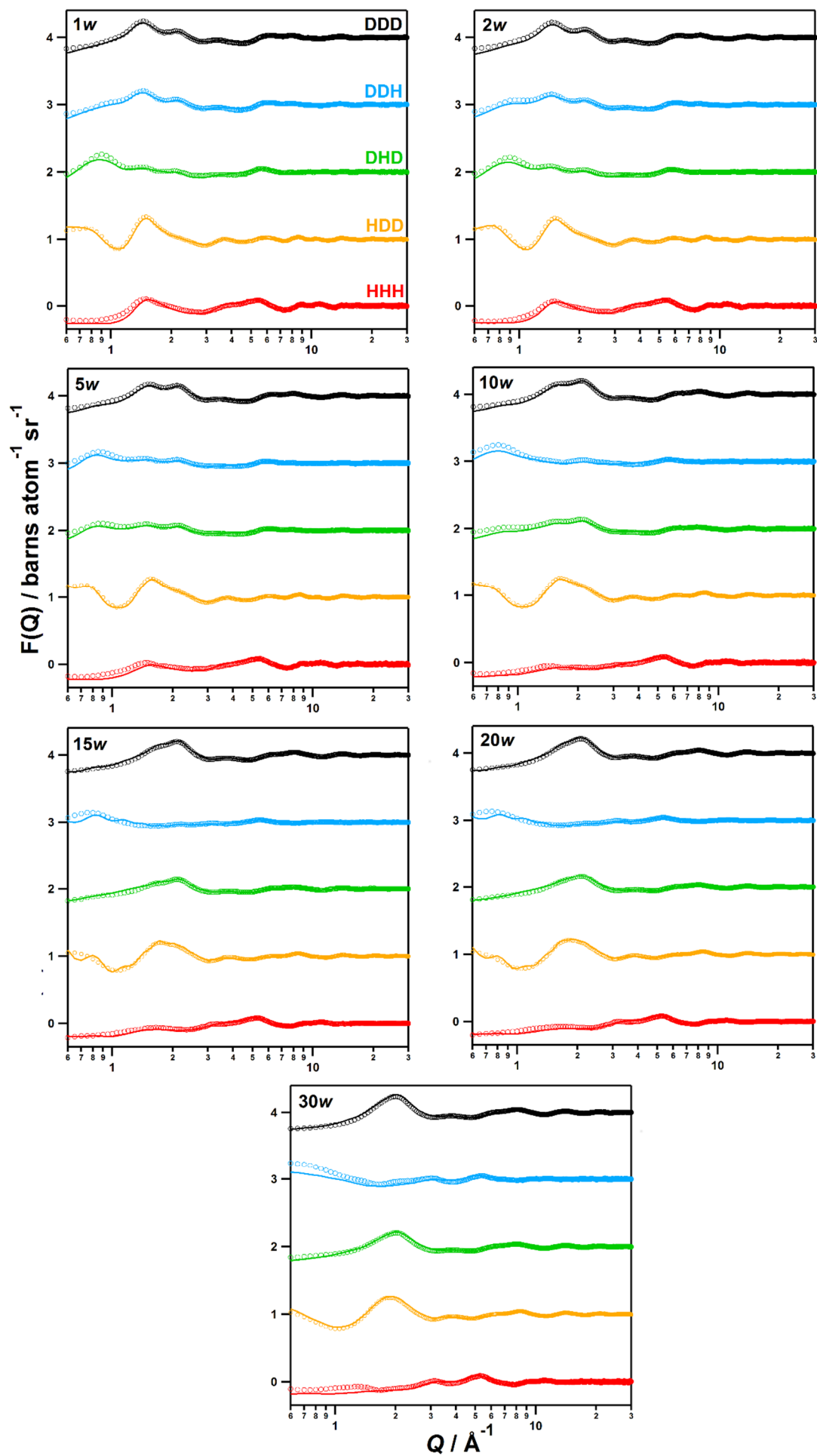
Figure 1. Corrected experimental neutron diffraction data (markers) and fits from Empirical Potential Structure Refinement atomistic models (solid lines) for the seven systems studied here.

3. Empirical Potential Structure Refinement (EPSR) modelling

Parameters for the water oxygen 'O_1' and hydrogen 'H_1' atoms were derived from the TIP3P model,[5] and are given in **Table 2**. The composition of each simulation box is shown in Table 3. The DES components of the hydrated EPSR models were parameterised and labelled in exactly the same way that was reported previously for the pure DES;[6] the atom labels are shown again for reference in Figure 2.

Table 2. EPSR parameters for water molecules that were used to model experimental diffraction data.

Atom type	ε / kJ mol^{-1}	σ / Å	q / e
O_1	0.634	3.151	-0.834
H_1	0.000	0.000	0.417

Table 3. The quantity of each molecule type used to build the simulation boxes is shown, alongside the total number of atoms in each box and the equilibrated box diameter. Atomic densities are calculated using a combination of literature values and experimental scattering data for H:H:H hydrated reline systems, and fall within the propagated errors from the literature measurements.[7]

Mixture	Choline	Chloride	Urea	Water	Total	Box diameter / Å	Density / atoms Å^{-3}
Reline-1w	400	400	800	400	2000	54.025	0.104005
Reline-2w	300	300	600	600	1800	50.166	0.104553
Reline-5w	200	200	400	1000	1800	46.710	0.104012
Reline-10w	150	150	300	1500	2100	46.355	0.102405
Reline-15w	100	100	200	1500	1900	43.353	0.101861
Reline-20w	100	100	200	2000	2400	45.824	0.101846
Reline-30w	100	100	200	3000	3400	50.651	0.098500
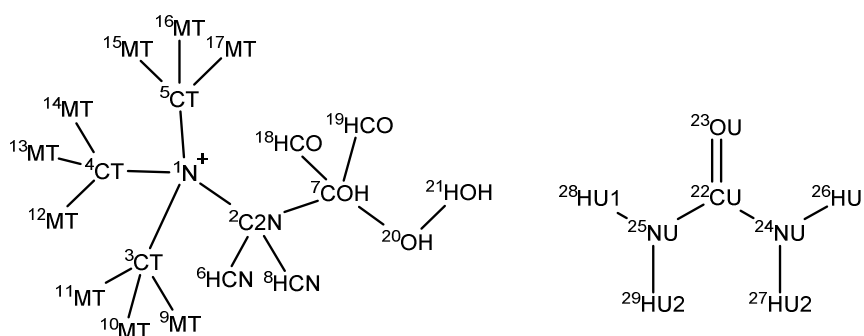
Figure 2. DES molecules used to create the EPSR reference potential. The shown atom type labels will be referred to in the text. Reprinted with permission from the Royal Society of Chemistry.[6]

Otherwise, the experimental procedure for the EPSR modelling was functionally identical to previous work on the pure reline DES.[6] The reference potential for each system was allowed to equilibrate to the experimental density described in Table 3, and the empirical potential was then allowed to equilibrate. Finally, ensemble information was interrogated from the model to gain information about the structure and bonding within these mixtures.

4. SDF plots

SDF plots are a way to aid with the visualisation of the 3D structure of a disordered liquid, with the surfaces showing the most likely places that a solvating species can be found around a certain molecule. Some additional spatial density function (SDF) plots are shown below, demonstrating some of the interesting and subtle changes occurring throughout the regime change. Firstly, the solvation of chloride by water is shown in supporting Figure 3, demonstrating the gradual increase in water-chloride interactions as the hydration level is increased. The appearance of the second solvation shell of chloride about water at 15w shows that water-chloride interactions are dominant over choline-chloride, and urea-chloride interactions. Secondly, the hydration of choline at 10w, the point at which this interaction is maximised, is shown in supporting Figure 4. Here, the water forms a radial solvation band around the choline, much like is seen in the pure solvent, for the choline-urea and choline-chloride interactions, but at closer length scale.

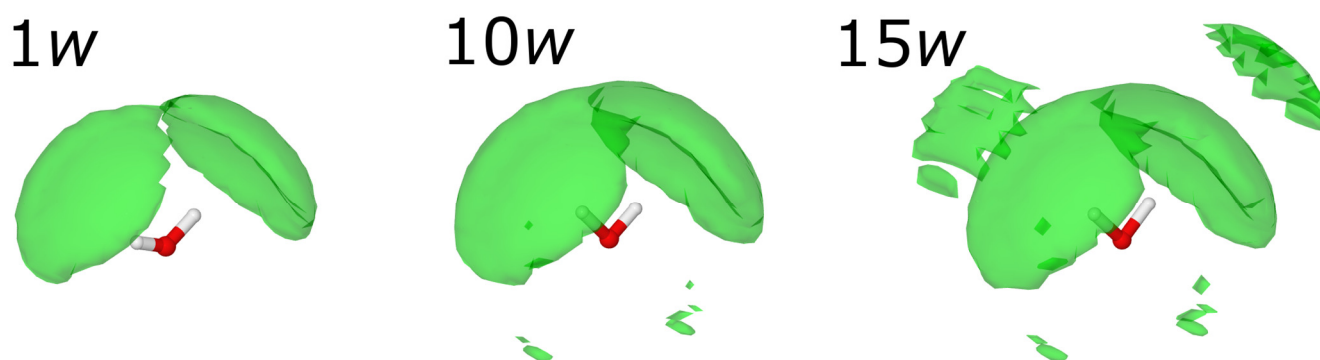Figure 3. SDF plots centered on water molecules at different hydration levels, showing their solvation by chloride (green surfaces), and plotted at the 7.5% probability level. As the hydration level increases, the water-chloride interaction becomes more prevalent.
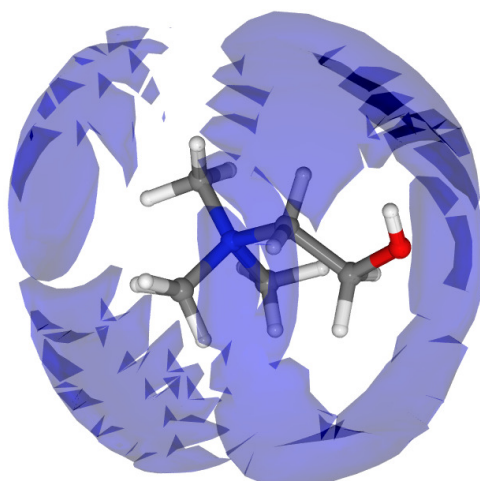

Figure 4. SDF plot showing hydration (blue surface) of choline at 10w, the point at which this interaction is maximised, and plotted at the 7.5% probability level.

5. Calculated Intermolecular Coordination Numbers

The tabulated intermolecular coordination numbers are shown in Tables 4 – 10, and these were calculated by integrating partial radial distribution functions (pRDFs) up to a radius R_{max} corresponding with their first minima, where R_{max} is accurate to a maximum of one data bin, *ie*. $R_{max} \pm 0.02$ A^{-1}. For these intermolecular coordination numbers the polyatomic molecular centres were defined as the C_{2N} atom of choline, the C_U atom of urea, and the O_1 atom of water.

Table 4. Calculated intermolecular coordination numbers for reline-1w. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	2.50	1.56
Urea	Water	4.9	1.48	1.20
Chloride	Water	4.5	1.18	1.08
Water	Water	4.0	0.91	0.97
Choline	Choline	7.8	4.58	1.64
Choline	Chloride	6.4	3.19	1.12
Choline	Chloride	4.7	1.04	0.78
Choline	Urea	6.8	6.69	2.18
Urea	Chloride	5.2	1.76	0.94
Urea	Urea	5.7	4.01	1.71

Table 5. Calculated intermolecular coordination numbers for reline-2*w*. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	4.81	2.22
Urea	Water	4.9	2.62	1.60
Chloride	Water	4.5	2.17	1.43
Water	Water	4.0	1.65	1.24
Choline	Choline	7.8	4.13	1.57
Choline	Chloride	6.4	3.01	1.14
Choline	Chloride	4.7	0.96	0.77
Choline	Urea	6.8	6.33	2.12
Urea	Chloride	5.2	1.60	0.92
Urea	Urea	5.7	3.67	1.62

Table 6. Calculated intermolecular coordination numbers for reline-5w. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	10.08	3.03
Urea	Water	4.9	5.28	2.06
Chloride	Water	4.5	4.24	1.83
Water	Water	3.3	1.83	1.08
Choline	Choline	7.8	3.34	1.56
Choline	Chloride	6.4	2.46	1.08
Choline	Chloride	4.7	0.77	0.71
Choline	Urea	6.8	4.88	1.89
Urea	Chloride	5.2	1.26	0.86
Urea	Urea	5.7	3.09	1.58

Table 7. Calculated intermolecular coordination numbers for reline-10w. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	15.37	3.08
Urea	Water	4.9	8.09	2.12
Chloride	Water	4.4	5.78	1.79
Water	Water	3.1	2.21	1.05
Choline	Choline	7.8	2.48	1.45
Choline	Chloride	6.4	1.87	1.03
Choline	Chloride	4.7	0.58	0.65
Choline	Urea	6.8	3.25	1.63
Urea	Chloride	5.2	0.90	0.78
Urea	Urea	5.7	2.39	1.36

Table 8. Calculated intermolecular coordination numbers for reline-15w. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	10.15	6.32
Urea	Water	4.9	7.61	3.90
Chloride	Water	4.3	5.21	3.09
Water	Water	3.0	2.64	1.27
Choline	Choline	8.2	4.37	2.53
Choline	Chloride	6.4	1.89	1.03
Choline	Chloride	4.7	0.59	0.65
Choline	Urea	6.8	3.23	1.79
Urea	Chloride	5.2	0.84	0.77
Urea	Urea	5.7	2.27	1.46

Table 9. Calculated intermolecular coordination numbers for reline-20w. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	14.18	5.44
Urea	Water	4.9	9.19	3.30
Chloride	Water	4.3	6.29	2.73
Water	Water	3.0	2.63	1.18
Choline	Choline	8.2	3.37	1.84
Choline	Chloride	6.4	1.50	0.99
Choline	Chloride	4.7	0.48	0.61
Choline	Urea	6.8	2.64	1.54
Urea	Chloride	5.2	0.67	0.69
Urea	Urea	5.7	1.78	1.27

Table 10. Calculated intermolecular coordination numbers for reline-30*w*. The calculated 'error' represents one standard deviation in coordination number.

Molecule A	Molecule B	R_{max} / Å	N_{coord}	±
Choline	Water	6.2	19.03	4.07
Urea	Water	4.9	10.84	2.50
Chloride	Water	4.2	6.69	1.91
Water	Water	3.0	2.68	1.09
Choline	Choline	8.2	2.05	1.48
Choline	Chloride	6.4	1.01	0.86
Choline	Chloride	4.7	0.32	0.51
Choline	Urea	6.8	1.56	1.17
Urea	Chloride	5.2	0.48	0.62
Urea	Urea	5.7	1.18	1.02

6. Integrated partial (site-site) coordination numbers

As with the intermolecular coordination numbers, the tabulated site-site radial distribution function analysis is shown in Tables 11 – 17. These values were calculated by integrating a selection of partial radial distribution functions (pRDFs) best describing the specific intermolecular bonding, up to a radius R_{max} corresponding with their first minima, where R_{max} is accurate to a maximum of one data bin, *ie*. $R_{max} \pm 0.02$ A^{-1}. For these coordination numbers, the 'error' reflects the disorder present in the liquid, rather than a lack of general confidence in the data. In this case, 'important' coordination numbers are those which have a variance significantly smaller than the coordination number itself, signifying a persistent correlation.

Table 11. Site-site coordination numbers calculated from selected pRDFs of reline-1w. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.0	3.25	1.49
Cl	N_U	3.9	3.10	1.67
Cl	H_{U1}	3.0	1.52	1.36
Cl	H_{U2}	3.0	1.02	0.93
H_{OH}	Cl	3.2	0.55	0.51
M_T	Cl	4.0	0.59	0.62
H_{CN}	Cl	4.0	0.59	0.61
H_{CO}	Cl	4.0	0.59	0.62
H_{CN}	O_U	3.5	0.48	0.62
M_T	O_U	3.4	0.52	0.65
H_{CO}	O_U	3.6	0.54	0.67
H_{OH}	O_U	2.5	0.19	0.40
H_{OH}	N_U	4.3	2.49	1.60
N	N	6.8	2.61	1.28
N	C_{2N}	7.5	4.98	1.58
N	C_{OH}	6.2	2.88	1.24
N	O_H	5.2	2.08	0.98
N	H_{OH}	5.5	2.36	1.10
O_U	N_U	3.5	3.31	1.05
O_U	H_{U1}	2.6	0.46	0.73
O_U	H_{U2}	2.6	1.73	0.87
N_U	H_{U1}	4.6	4.87	2.01
N_U	H_{U2}	4.6	4.97	1.78
Cl	Cl	6.0	1.23	0.91
N	O_1	5.8	2.09	1.41
H_{OH}	O_1	2.3	0.07	0.26
H_{CN}	O_1	3.5	0.28	0.52
H_{CO}	O_1	3.6	0.32	0.56
Cl	O_1	4.3	1.09	1.03
O_1	O_1	4.2	0.99	1.02

Table 12. Site-site coordination numbers calculated from selected pRDFs of reline-2*w*. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.0	2.93	1.40
Cl	N_U	3.9	2.77	1.59
Cl	H_{U1}	3.0	1.38	1.32
Cl	H_{U2}	3.0	0.89	0.86
H_{OH}	Cl	3.2	0.53	0.51
M_T	Cl	4.0	0.54	0.61
H_{CN}	Cl	4.0	0.55	0.60
H_{CO}	Cl	4.0	0.54	0.61
H_{CN}	O_U	3.5	0.45	0.61
M_T	O_U	3.4	0.48	0.63
H_{CO}	O_U	3.6	0.50	0.64
H_{OH}	O_U	2.5	0.17	0.38
H_{OH}	N_U	4.3	2.34	1.55
N	N	6.8	2.27	1.23
N	C_{2N}	7.5	4.53	1.50
N	C_{OH}	6.2	2.66	1.16
N	O_H	5.2	1.96	0.92
N	H_{OH}	5.6	2.29	1.06
O_U	N_U	3.5	3.19	1.01
O_U	H_{U1}	2.6	0.42	0.70
O_U	H_{U2}	2.6	1.72	0.85
N_U	H_{U1}	4.6	4.58	1.92
N_U	H_{U2}	4.6	4.69	1.71
Cl	Cl	6.0	1.14	0.90
N	O_1	5.6	3.65	1.90
H_{OH}	O_1	2.3	0.14	0.35
H_{CN}	O_1	3.5	0.53	0.70
H_{CO}	O_1	3.6	0.62	0.77
Cl	O_1	4.3	1.99	1.36
O_1	O_1	4.0	1.65	1.24

Table 13. Site-site coordination numbers calculated from selected pRDFs of reline-5w. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.1	2.40	1.35
Cl	N_U	4.0	2.28	1.53
Cl	H_{U1}	3.0	1.08	1.17
Cl	H_{U2}	3.0	0.65	0.77
H_{OH}	Cl	3.2	0.43	0.50
M_T	Cl	4.0	0.42	0.55
H_{CN}	Cl	4.0	0.44	0.56
H_{CO}	Cl	4.0	0.43	0.56
H_{CN}	O_U	3.5	0.33	0.54
M_T	O_U	3.4	0.36	0.55
H_{CO}	O_U	3.6	0.37	0.56
H_{OH}	O_U	2.5	0.13	0.35
H_{OH}	N_U	4.3	1.78	1.42
N	N	6.8	1.76	1.16
N	C_{2N}	7.5	3.85	1.49
N	C_{OH}	6.2	2.32	1.11
N	O_H	5.3	1.81	0.88
N	H_{OH}	5.6	2.01	0.98
O_U	N_U	3.5	2.96	0.96
O_U	H_{U1}	2.6	0.33	0.64
O_U	H_{U2}	2.6	1.58	0.83
N_U	H_{U1}	4.6	4.13	1.83
N_U	H_{U2}	4.6	4.19	1.65
Cl	Cl	6.0	0.85	0.80
N	O_1	5.4	6.82	2.41
H_{OH}	O_1	2.3	0.25	0.44
H_{CN}	O_1	3.6	1.13	0.95
H_{CO}	O_1	3.6	1.23	1.01
Cl	O_1	4.3	3.83	1.71
O_1	O_1	3.5	2.07	1.16

Table 14. Site-site coordination numbers calculated from selected pRDFs of reline-10w. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.2	1.79	1.24
Cl	N_U	4.1	1.71	1.39
Cl	H_{U1}	3.0	0.76	1.00
Cl	H_{U2}	3.0	0.44	0.65
H_{OH}	Cl	3.2	0.35	0.48
M_T	Cl	4.0	0.30	0.49
H_{CN}	Cl	4.0	0.33	0.51
H_{CO}	Cl	4.0	0.32	0.51
H_{CN}	O_U	3.5	0.22	0.45
M_T	O_U	3.5	0.25	0.47
H_{CO}	O_U	3.6	0.27	0.49
H_{OH}	O_U	2.5	0.10	0.30
H_{OH}	N_U	4.3	1.21	1.19
N	N	7.3	1.88	1.25
N	C_{2N}	7.7	3.41	1.43
N	C_{OH}	6.4	2.09	1.01
N	O_H	5.4	1.62	0.77
N	H_{OH}	5.8	1.84	0.90
O_U	N_U	3.6	2.78	0.89
O_U	H_{U1}	2.6	0.25	0.55
O_U	H_{U2}	2.6	1.51	0.77
N_U	H_{U1}	4.6	3.49	1.60
N_U	H_{U2}	4.6	3.57	1.45
Cl	Cl	6.0	0.58	0.69
N	O_1	5.4	10.12	2.42
H_{OH}	O_1	2.3	0.35	0.48
H_{CN}	O_1	3.6	1.61	1.05
H_{CO}	O_1	3.6	1.75	1.12
Cl	O_1	4.2	5.12	1.66
O_1	O_1	3.4	2.70	1.16

Table 15. Site-site coordination numbers calculated from selected pRDFs of reline-15w. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.2	1.67	1.25
Cl	N_U	4.2	1.75	1.50
Cl	H_{U1}	3.0	0.77	1.05
Cl	H_{U2}	3.0	0.43	0.65
H_{OH}	Cl	3.2	0.38	0.49
M_T	Cl	4.0	0.32	0.50
H_{CN}	Cl	4.1	0.36	0.52
H_{CO}	Cl	4.1	0.37	0.53
H_{CN}	O_U	3.6	0.26	0.49
M_T	O_U	3.5	0.26	0.49
H_{CO}	O_U	3.6	0.27	0.50
H_{OH}	O_U	2.5	0.12	0.33
H_{OH}	N_U	4.3	1.28	1.26
N	N	7.7	3.58	2.22
N	C_{2N}	8.0	5.10	2.43
N	C_{OH}	6.7	3.06	1.56
N	O_H	5.5	2.05	1.07
N	H_{OH}	6.0	2.47	1.32
O_U	N_U	3.8	2.94	1.03
O_U	H_{U1}	2.6	0.26	0.57
O_U	H_{U2}	2.6	1.52	0.78
N_U	H_{U1}	4.6	3.44	1.69
N_U	H_{U2}	4.6	3.46	1.52
Cl	Cl	6.0	0.48	0.63
N	O_1	5.5	7.00	4.49
H_{OH}	O_1	2.3	0.25	0.44
H_{CN}	O_1	3.6	0.99	1.08
H_{CO}	O_1	3.6	1.09	1.17
Cl	O_1	4.1	4.59	2.73
O_1	O_1	3.3	3.59	1.56

Table 16. Site-site coordination numbers calculated from selected pRDFs of reline-20*w*. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.3	1.39	1.14
Cl	N_U	4.2	1.39	1.32
Cl	H_{U1}	3.0	0.62	0.91
Cl	H_{U2}	3.0	0.33	0.56
H_{OH}	Cl	3.2	0.29	0.46
M_T	Cl	4.0	0.25	0.46
H_{CN}	Cl	4.1	0.29	0.48
H_{CO}	Cl	4.1	0.28	0.48
H_{CN}	O_U	3.6	0.21	0.44
M_T	O_U	3.6	0.23	0.46
H_{CO}	O_U	3.6	0.22	0.45
H_{OH}	O_U	2.6	0.11	0.32
H_{OH}	N_U	4.5	1.28	1.29
N	N	8.0	3.10	1.74
N	C_{2N}	8.3	4.48	1.85
N	C_{OH}	6.8	2.69	1.29
N	O_H	5.6	1.90	0.94
N	H_{OH}	6.2	2.30	1.14
O_U	N_U	3.9	2.80	0.95
O_U	H_{U1}	2.6	0.20	0.50
O_U	H_{U2}	2.6	1.46	0.75
N_U	H_{U1}	4.6	3.02	1.47
N_U	H_{U2}	4.6	3.04	1.37
Cl	Cl	6.0	0.36	0.57
N	O_1	5.6	10.29	4.11
H_{OH}	O_1	2.3	0.34	0.48
H_{CN}	O_1	3.6	1.35	1.14
H_{CO}	O_1	3.6	1.50	1.22
Cl	O_1	4.1	5.51	2.41
O_1	O_1	3.3	3.56	1.40

Table 17. Site-site coordination numbers calculated from selected pRDFs of reline-30w. The calculated 'error' represents one standard deviation in coordination number.

Atom A	Atom B	R_{max} / Å	N_{coord}	±
Cl	C_U	5.4	1.05	0.96
Cl	N_U	4.4	1.12	1.19
Cl	H_{U1}	3.1	0.49	0.83
Cl	H_{U2}	3.1	0.25	0.49
H_{OH}	Cl	3.2	0.21	0.40
M_T	Cl	4.0	0.17	0.38
H_{CN}	Cl	4.1	0.20	0.42
H_{CO}	Cl	4.2	0.20	0.41
H_{CN}	O_U	3.6	0.13	0.35
M_T	O_U	3.6	0.14	0.37
H_{CO}	O_U	3.6	0.12	0.34
H_{OH}	O_U	2.6	0.06	0.23
H_{OH}	N_U	4.4	0.66	0.93
N	N	8.2	2.04	1.43
N	C_{2N}	8.6	3.32	1.56
N	C_{OH}	6.8	2.04	1.09
N	O_H	5.6	1.56	0.78
N	H_{OH}	6.3	1.82	0.95
O_U	N_U	3.9	2.52	0.78
O_U	H_{U1}	2.6	0.13	0.40
O_U	H_{U2}	2.6	1.35	0.70
N_U	H_{U1}	4.6	2.48	1.23
N_U	H_{U2}	4.6	2.53	1.13
Cl	Cl	6.0	0.25	0.48
N	O_1	6.0	17.01	3.63
H_{OH}	O_1	2.3	0.47	0.51
H_{CN}	O_1	3.6	1.80	1.14
H_{CO}	O_1	3.6	1.97	1.22
Cl	O_1	4.1	6.24	1.82
O_1	O_1	3.3	3.52	1.22

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